



Screen the best ionic liquids for keratin dissolution by using COSMO-RS

Liu, Xue; Nie, Yi; Zhang, Suojia; Skov, Anne Ladegaard

Publication date:
2018

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):

Liu, X., Nie, Y., Zhang, S., & Skov, A. L. (2018). *Screen the best ionic liquids for keratin dissolution by using COSMO-RS*. Abstract from 8th International Conference on Electromechanically Active Polymer (EAP) Transducers & Artificial Muscles (EuroEAP 2018), Lyon, France.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.



EuroEAP 2018

International conference on
Electromechanically Active Polymer (EAP)
transducers & artificial muscles
Lyon, France, 5-6 June 2018

Organized and supported by
"European Scientific Network for Artificial
Muscles – ESNAM" (www.esnam.eu)
COST Action MP1003



Screen the best ionic liquids for keratin dissolution by using COSMO-RS

Xue Liu (1)(2), Yi Nie(2), Suojiang Zhang (2)*, Anne Ladegaard Skov(1)*

- (1) Danish Polymer Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark;
(2) CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China;

Wool keratin is a kind of degradable natural biopolymer and extensively used in the textile and biomedical fields. But keratin is hard to reuse because it is difficult to dissolve in conventional solvents. An increasing interest has been manifested in the use of ionic liquids (ILs) as solvents for dissolution of wool keratin due to their tuneable and excellent properties. However, it is nevertheless a challenge to identify the best ILs for keratin dissolution. Experimental measurement of all these systems is not practically feasible; hence a rapid and a priori screening method to predict the keratin solubility capacity for ILs is needed. Based on our previous work, we designed three models for describing wool keratin, and 462 ILs formed from 21 cations and 22 anions were selected for evaluation of their ability to dissolve wool keratin by COSMO-RS. From the prediction results of logarithmic activity coefficients ($\ln\gamma$) of the three keratin models, it can be concluded that keratin dissolution capacity is mostly determined by the anion while the cation only has a moderate effect on the dissolution process. Ac^- , Dec^- , HCOO^- , Cl^- , BEN^- , DMP^- , DEP^- , DBP^- , TOS^- and Br^- with various cations studied in this work exhibited particularly good properties for keratin dissolution. The excess enthalpy calculations indicated that the main forces in the keratin dissolution in ILs are H-bonds, while the contribution of misfit forces and van der Waals forces are secondary.

References

1. Zhang, Z., Nie, Y., Zhang, Q., Liu, X., Tu, W., Zhang, X., & Zhang, S. (2017). Quantitative Change in Disulfide Bonds and Microstructure Variation of Regenerated Wool Keratin from Various Ionic Liquids. *ACS Sustainable Chemistry & Engineering*, 5(3), 2614-2622.
2. Liu, X., Nie, Y., Meng, X., Zhang, Z., Zhang, X., & Zhang, S. (2017). DBN-based ionic liquids with high capability for the dissolution of wool keratin. *RSC Advances*, 7(4), 1981-1988.
3. Idris, A., Vijayaraghavan, R., Rana, U. A., Patti, A. F., & MacFarlane, D. R. (2014). Dissolution and regeneration of wool keratin in ionic liquids. *Green Chemistry*, 16(5), 2857-2864.
4. Zheng, S., Nie, Y., Zhang, S., Zhang, X., & Wang, L. (2015). Highly efficient dissolution of wool keratin by dimethylphosphate ionic liquids. *ACS Sustainable Chemistry & Engineering*, 3(11), 2925-2932.
5. Idris, A., Vijayaraghavan, R., Rana, U. A., Fredericks, D., Patti, A. F., & MacFarlane, D. R. (2013). Dissolution of feather keratin in ionic liquids. *Green chemistry*, 15(2), 525-534.